School of Chemistry

Aims and Objectives: Session 2022-2023

Module CH5714: Chemical Applications of Electronic Structure Calculations

Duration: 20 hours

Lecturers: Professor M. Bühl* and Dr J. B. O. Mitchell

(*Module Convenor)

Aims: The course will build on the foundations laid in the modules CH2701 and CH3712 and discuss further aspects and methods of modern computational chemistry related to the electronic structures of atoms and molecules. It will be shown how results of such calculations can be used to complement, interpret, and guide experiments in many areas of chemistry.

Objectives:

1. To provide an overview of *ab initio* methods and their associated "model chemistries".

2. To discuss density functional theory and give an overview of its current state-of-the-art.

3. To consider applications of computed structures and energies in chemistry.

4. To discuss both the theoretical underpinnings and the applications of molecular dynamics simulations.

5. To give an overview of the theory of intermolecular forces.

6. To discuss the development of force fields and their applications in molecular simulations.